The spin-Peierls instability in spin 1/2 XY chain
in the non adiabatic limit

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Abstract

The spin-Peierls instability in spin 1/2 XY chain coupled to dispersionless phonons of frequency ω has been studied in the nonadiabatic limit. We have chosen the Lang-Firsov variational wave function for the phonon subsystem to obtain an effective spin Hamiltonian. The effective spin Hamiltonian is then solved in the framework of mean-field approximation. We observed a dimerized phase when g is less than a critical value and an anti-ferromagnetic phase when it is greater than a critical value . The variation of lattice distortion, dimerized order parameter and energy gap with spin phonon coupling parameter has also been investigated here.

1. Introduction

The discovery of the spin Peierls transition in $CuGeO_3$ [1] has sparked an intense effort to study the properties of this quasi one-dimensional magneto-elastic system where the coupling of the magnetic to the lattice degrees of freedom leads to a phase transition into a dimerized phase. This magneto elastic transition is due to the competition between the gain in magnetic energy due to dimerization and the loss in the elastic energy of the lattice distortion. Recently quite a large number of experimental [2–5] and theoretical [6–13] works have been performed to investigate the various aspects of the spin Peierls systems. Except a few [14,15] most of the theoretical investigations rely on the adiabatic treatment of the phonons. In adiabatic approaches one assumes that the phonons responsible for the distortion have low energy with respect to the characteristic energies for the spin systems (e.g. the gap=Δ). The experimental evidence for $CuGeO_3$ indicates that the application of the adiabatic approximation to these system is not sufficient. Regnault et al. [16] investigated the spin dynamics of spin Peierls system $CuGeO_3$ by inelastic neutron scattering. Their result confirmed the existence of a gap (Δ) in the magnetic excitations at $\Delta = 2meV = 23K$ and the Heisenberg exchange parameter was considered to be $J_1 = 10.6meV = 115K$. Braden et al. [17] found by symmetry that four optical phonons are possible candidates for the spin Peierls distortion in $CuGeO_3$. Among these four modes

two, one of energy 330^oK and other of energy 150^oK are experimentally found to be the suitable candidates for the spin Peierls distortion. In both cases we find that the phonon frequency is larger than J as well as Δ. When $\omega > \Delta$ the spin phonon interaction is unretarded and non-adiabatic effects or quantum lattice fluctuations become important. Fradkin and Hirsch [18] considered the Su-Schrieffer-Heeger model [19] of electron-phonon interaction for spin-less fermions and spin $\frac{1}{2}$ electrons in one dimension to investigate the stability of the Peierls-dimerized ground state against quantum fluctuations. In this work they have shown by renormalization group arguments and by quantum Monte Carlo simulation that for spin-less fermions quantum lattice fluctuations destroy the long-range dimerization order when the fermion-phonon coupling constant is small and predicted a transition from an undimerized ground state to a dimerized phase when the fermion-phonon interaction is larger than a critical value. Campbell and Bishop [20] independently confirmed the findings of Fradkin and Hirsch. Recently Caron and Moukouri [14] studied the XY spin chain coupled to dispersionless phonons by the density matrix renormalisation group (DMRG) method and showed that quantum fluctuations reduce the spin Peierls gap and even destroy the dimerization when the phonon frequency gets appreciably larger than the gap.

The coupled spin-phonon system for all values of the coupling parameter is a very difficult problem. However, one may gain considerable insight into the stability problem by simply considering limiting situations. By analyzing the stability of these limits a qualitative picture of possible phases (or the ground state) will emerge. In the present work we will investigate the effect of spin-phonon interaction in the non-adiabatic limit i.e. when phonons are certainly fast. In this case we will treat the phonons as fast variables and derive an effective interacting fermion model.

We propose to study an XY spin chain whose magnetic interaction depends on the bond length. The reason for this study is two fold i) The undeformed spin chain Hamiltonian can be solved exactly.

ii) The model contains the essential elements for the spin-Peierls transition, that is coupling to intermolecular motion. In the future it will be of interest to study the Heisenberg chain with next-nearest neighbor frustration term to make the model more realistic to the inorganic spin-Peierls systems.

The paper is organized as follows. In section 2 the variational ground state energy of the XY model in presence of spin-phonon interaction is determined using suitable phonon states and mean field approximation taking into account the dimerization as well as anti-ferromagnetic ordering. The results of numerical solution and its implication are discussed in section 3.

2. Formulation

We start with the XY model in presence of spin phonon interaction on a linear chain:

$$H = \sum_l [(J + g(b_l^\dagger + b_l - b_{l+1}^\dagger - b_{l+1})](S_l^X S_{l+1}^X + S_l^Y S_{l+1}^Y) + \omega \sum_l b_l^\dagger b_l \tag{1}$$

where l denotes the site index of the N site linear chain, S_l^X and S_l^Y are components of the local X-Y spin of value $\frac{1}{2}$, $b_l(b_l^\dagger)$ is the annihilation (creation) operator for a vibration of molecule at site l and J is the magnetic exchange interaction between the nearest neighbor spins. Here ω accounts for the dispersionless vibrational spectra for molecular motion along the chain direction and g is the spin-phonon interaction [21].

We transform the spin operator to a spinless pseudo fermion representation using the Jordan Wigner transformation [22]

$$S_l^X + iS_l^Y = S_l^+ = exp(-i\pi \sum_j^{l-1} d_j^\dagger d_j) d_l^\dagger, \tag{2}$$

$$S_l^X - iS_l^Y = S_l^- = exp(i\pi \sum_j^{l-1} d_j^\dagger d_j) d_l, \tag{3}$$

$$S_l^z = \frac{1}{2} + d_l^\dagger d_l \tag{4}$$

to make use of the growing understanding of one dimensional Fermi system.

After the Jordan Wigner transformation the Hamiltonian (1) can be written in terms of fermion operators $d_l^\dagger$ and d_l as

$$H = \frac{1}{2}J \sum_l P_l + \frac{1}{2}g \sum_l (b_l^\dagger + b_l)(P_l - P_{l-1}) + \omega \sum_l b_l^\dagger b_l \tag{5}$$

where

$$P_l = d_l^\dagger d_{l+1} + d_{l+1}^\dagger d_l. \tag{6}$$

In the adiabatic approximation the spin-phonon interaction deforms the lattice to undergo the Peierls instability. To take into account the lattice distortion due to spin phonon coupling in our case we choose a variational wave function $|\psi\rangle_{ph} = U|0\rangle$ with

$$U = exp(\frac{\lambda}{2\omega} \sum_l (b_l^\dagger - b_l)(P_l - P_{l-1})) \tag{7}$$

for the phonon subsystem, where $|0\rangle$ is the zero phonon state and U describes a modified Lang-Firsov transformation [23,24]. In this formalism the effective fermion Hamiltonian is written as

$$H_{eff} = \langle 0|H_T|0\rangle, \tag{8}$$

with

$$H_T = U^{-1}HU$$

$$= \frac{J}{2}\sum_l U^{-1}P_l U + \frac{g-\lambda}{2}\sum_l (b_l^\dagger + b_l)(P_l - P_{l-1})$$

$$- 4g'^2 \sum_l n_l + 4g'^2 \sum_l n_l n_{l+1} + g'^2 \sum (1 - 2n_l)(d_{l-1}^\dagger d_{l+1} + d_{l+1}^\dagger d_{l-1})$$

$$+ \omega \sum_l b_l^\dagger b_l \tag{9}$$

where,

$$n_l = d_l^\dagger d_l, \tag{10}$$

$$g'^2 = (\frac{g\lambda}{2\omega} - \frac{\lambda^2}{4\omega}). \tag{11}$$

In the above equation b_l and $b_l^\dagger$ is the creation and annihilation operator for the phonon system vibrating about the displaced equilibrium position $\frac{\lambda}{\omega}(P_l - P_{l-1})$ of the lattice. Clearly, λ is proportional to a lattice displacement created by the spin-phonon interaction which has to be determined variationally. When $\lambda = g$ the transformation is exactly the Lang-Firsov [23] transformation where the fermion-phonon term is diagonalised exactly and the fermion hopping term is renormalized by dressed phonons. To obtain an effective fermionic Hamiltonian we take the average over the zero phonon state of the transformed phonon subsystem and neglect the terms of the order of $\frac{\lambda^4}{\omega^4}$ and higher. In this approximation the effective Hamiltonian is

$$H_{eff}(\lambda) = \frac{J}{2}(1 - \frac{3\lambda^2}{4\omega^2})\sum_l (d_l^\dagger d_{l+1} + d_{l+1}^\dagger d_l) + \frac{J\lambda^2}{8\omega^2}\sum_l (d_l^\dagger d_{l+3} + d_{l+3}^\dagger d_l)$$

$$- 4g'^2 \sum_l n_l + 4g'^2 \sum_l n_l n_{l+1} + g'^2 \sum (1 - 2n_l)(d_{l-1}^\dagger d_{l+1} + d_{l+1}^\dagger d_{l-1})$$

$$+ O(\lambda^4). \tag{12}$$

Now, the above effective hamiltonian (12) is complicated enough to solve it exactly. Therefore one has to look for the approximate methods. We calculate the ground state energy $E_{eff}(\lambda)$ of the effective Hamiltonian (13) in the framework of mean field theory. We assume solutions which break the symmetry between even and odd sites with respect to the number of fermions on the site and to the corresponding hopping probability. Both of these kinds of oder open a gap at the Fermi momentum at half filling (ie. when the total spin M_z is zero) and lower the ground state energy. We will consider four variational parameters such as n_e, n_o, h_e and h_o (where, e implies even sites and o implies odd sites). All these variables are not independent because they are subject to the fermion number conservation constraint

$$n = \frac{< d_{2l}^\dagger d_{2l} + d_{2l+1}^\dagger d_{2l+1} >}{2} = \frac{(n_e + n_o)}{2} \tag{13}$$

For half filling ($M_z = 0$) $n = \frac{1}{2}$. The three remaining variational parameters are then the anti-ferromagnetic order parameter

$$m = \frac{< d_{2l}^\dagger d_{2l} - d_{2l+1}^\dagger d_{2l+1} >}{2} = \frac{(n_e - n_o)}{2}, \tag{14}$$

the dimerized order parameter

$$\gamma = \frac{< d_{2l}^\dagger d_{2l+1} - d_{2l+1}^\dagger d_{2l+2} >}{2} = \frac{(h_e - h_o)}{2} \tag{15}$$

and average hopping probability

$$h = \frac{< d_{2l}^\dagger d_{2l+1} + d_{2l+1}^\dagger d_{2l+2} >}{2} = \frac{(h_e + h_o)}{2} \tag{16}$$

Here $< --- >$ implies the expectation value over the ground state. Within the limitation of Hartree-Fock approximation our effective Hamiltonian can be written as

$$
\begin{aligned}
H_{eff} = {} & \frac{J}{2}(1 - \frac{3\lambda^2}{4\omega^2}) \sum_l (d_l^\dagger d_{l+1} + d_{l+1}^\dagger d_l) + \frac{J\lambda^2}{8\omega^2} \sum_l (d_l^\dagger d_{l+3} + d_{l+3}^\dagger d_l) \\
& + 8g'^2 \gamma \sum_l (-1)^l (d_l^\dagger d_{l+1} + d_{l+1}^\dagger d_l) + 8g'^2 \sum (\frac{1}{2} - (-1)^l m) n_l) \\
& - 4g'^2(\frac{1}{4} - m^2 - 2\gamma^2)N - 2g'^2 N + O(\frac{\lambda^4}{\omega^4})
\end{aligned} \tag{17}
$$

To diagonalise the Hamiltonian (18) we transform the operators from coordinate space to momentum space

$$c_j^\dagger = \frac{1}{\sqrt{N}} \sum_k c_k^\dagger e^{ikj} \tag{18}$$

$$c_j = \frac{1}{\sqrt{N}} \sum_k c_k e^{-ikj} \tag{19}$$

Due to the reduced symmetry each k state is coupled to the state $k + \pi$. So it is convenient to write the Hamiltonian in the reduced zone $-\frac{\pi}{2}$ to $\frac{\pi}{2}$ and label the states by band indices l and u. In this representation the Hamiltonian is a two band Hamiltonian where the band l and u are coupled to each k.

$$
\begin{aligned}
H_{eff} = {} & \sum_k \alpha_k^l d_k^{l\dagger} d_k^l + \sum_k \alpha_k^u d_k^{u\dagger} d_k^u + \sum_k \beta_k d_k^{l\dagger} d_k^u + \sum_k \beta_k^* d_k^{u\dagger} d_k^l \\
& - 4g'^2(\frac{1}{4} - m^2 - 2\gamma^2)N + O(\frac{\lambda^4}{\omega^4})
\end{aligned} \tag{20}
$$

where,

$$\alpha_k^l = J(1 - \frac{3\lambda^2}{4\omega^2})cos(k) + \frac{2J\lambda^2}{8\omega^2}cos(3k) \tag{21}$$

$$\alpha_k^u = -J(1 - \frac{3\lambda^2}{4\omega^2})cos(k) - \frac{2J\lambda^2}{8\omega^2}cos(3k) \tag{22}$$

$$\beta_k = -8g'^2(m - 2i\gamma sin(k)) \tag{23}$$

We diagonalise this Hamiltonian by a Bogoliubov Valatin transformation and obtain

5

$$\frac{H_{eff}}{\omega} = \sum_k E_k^l a_k^\dagger a_k + \sum_k E_k^u b_k^\dagger b_k$$

$$- 4g'^2(\frac{1}{4} - m^2 - 2\gamma^2)N \tag{24}$$

with upper and lower band

$$E_k^{u/l} = \pm\sqrt{\frac{\alpha_k^{l2}}{\omega^2} + 64\frac{g'^4 m^2}{\omega^2} + \frac{256 g'^4 \gamma^2 sin(k)^2}{\omega^2}} \tag{25}$$

From the equation (25) it is clear that the energy spectrum has been split into two separate bands (for non zero m or γ) characterized by the Bogoliubov transformed creation (annihilation) operators $a_k^\dagger(a_k)$ and $b_k^\dagger(b_k)$. For half-filling ($M_z = 0$) the lower band is completely filled in the ground state . We will take the expectation value of the equations (14) (15) over the ground state to obtain a set of self-consistent equations of

$$m = 8\frac{g'^2 m}{\omega N} \sum_{k=-\pi/2}^{k=\pi/2} \frac{1}{|E_k^l|} \tag{26}$$

and

$$\gamma = 16\frac{g'^2\gamma}{\omega N} \sum_{k=-\pi/2}^{k=\pi/2} \frac{sin(k)^2}{|E_k^l|} \tag{27}$$

If we retain terms up to the order of $\frac{g^2}{\omega^2}$ the integrals involving the equations (26) and (27) can be expressed in terms of elliptic functions of the first kind $(K(\nu))$ and the second kind $(E(\nu))$ to give

$$m = \frac{8g'^2 \sqrt{\nu}\, m}{\pi J(1 - \frac{3\lambda^2}{2\omega^2})} K(\nu) \tag{28}$$

with $\nu = \frac{1}{1+\frac{64g'^4 m^2}{J^2(1-3\lambda^2/(2\omega^2))}}$ and

$$\gamma = -\frac{32g'^2\gamma}{\pi J(1 - \frac{3\lambda^2}{2\omega^2})} \frac{d}{d\nu'} E(\nu') \tag{29}$$

and $\nu' = 1 - \frac{256g'^4\gamma^2}{J^2(1-3\lambda^2/(2\omega^2))}$. For small m or γ the equations provide asymptotic expressions for 1) the antiferromagnetic and 2) the dimerized phase.

1) The antiferromagnetic phase $(\gamma = 0; m \neq 0)$

$$\gamma = 0;$$

$$m = p_j exp(-\pi p_j(1 - \frac{1.38629}{p_j}) \tag{30}$$

2) The dimerized phase $(m = 0; \gamma \neq 0)$

$$m = 0;$$

$$\gamma = \frac{pj}{2} exp(-\frac{\pi pj}{2}(1 - \frac{0.77308}{pj}) \tag{31}$$

where $p_j = J\frac{1-3\lambda^2/(2\omega^2)}{8g'^2}$

When m or γ is large we solve the equation (26) or (27) numerically to get the anti-ferromagnetic or dimerized order parameter.

Finally we minimize the ground state energy $(E_G(\lambda))$ of the Hamiltonian H_{eff} with respect to λ to get λ and the ground state energy of the system.

3. Results and discussion

We have computed the ground state energy, the lattice distortion and the energy gap for the XY system in presence of spin-phonon interaction when phonon frequency is certainly fast. The results of our calculation shows some distinguished features in the phase diagram which is absent when phonons are treated adiabatically. In the adiabatic approach the spin-phonon coupling to the XY spin system always gives rise to dimerized phase where as our nonadiabatic approach predicts spin-liquid, dimerized and antiferromagnetic phase depending on the values of $\frac{g}{\omega}$ and $\frac{J}{\omega}$ ratio. Here we present the result for two values for exchange interaction $\frac{J}{\omega} = 0.2$ and 0.4. In our calculation we have neglected the terms of the order $\frac{\lambda^4}{\omega^4}$ or higher. So we do not extend our calculation for large spin-phonon coupling $\frac{g}{\omega}$ and confine ourselves to $\frac{g}{\omega} \leq 0.5$. In figure 1. we have shown the variation of lowest energy in the anti-ferromagnetic as well as dimerized phase to determine the ground state of the system. For $\frac{J}{\omega} = 0.2$ we find that the dimerized phase represents the ground state when $\frac{g}{\omega} < .46$ and anti-ferromagnetic phase becomes the ground state when $\frac{g}{\omega} > 0.46$. The critical value for dimerized to anti-ferromagnetic phase transition increases with the increase of $\frac{J}{\omega}$. For J=0.4 the above mentioned critical value of $\frac{g}{\omega}$ is higher than 0.5 and it is not shown in our plot because we have confined our investigations within $\frac{g}{\omega} = 0.5$.

In figure 2. we show the variation of dimerized order parameter γ with $\frac{g}{\omega}$ for $\frac{J}{\omega} = 0.2$ and 0.4. The figure shows that when $\frac{g}{\omega}$ is less than 0.1 the dimerized order parameter is almost zero. From the equation (31) we obtain $\gamma \sim 10^{-20}$ at $\frac{g}{\omega} = 0.1$. In the mean-field calculation we neglect quantum fluctuations and always find a nonzero value of the order parameter. However, the quantum fluctuation due to spin excitation would have drastic repercussions on the value of γ and can destroy this small value of γ to give a spin liquid phase. So one may expect a critical spin-phonon coupling $(\frac{g_c}{\omega})$ for the on set of dimerization. Caron and Moukouri [14] have shown this existence of critical spin - phonon coupling $(\frac{g_c}{\omega})$ through the density matrix renormalization group calculation where quantum fluctuation are taken into account rigorously. It is also evident from our figure 2. that the dimerization order parameter decreases with the increase of $\frac{J}{\omega}$ which means that we expect a larger $\frac{g_c}{\omega}$ for $\frac{J}{\omega} = 0.4$.

Due to Peierls instability we have two types of bond length one is greater than the unperturbed lattice constant and other is less than the unperturbed lattice constant. We represent this lattice deformation by $< b_l^\dagger + b_l - b_{l+1}^\dagger - b_{l+1} >=$

$(-1)^l \delta$. In figure 3. we plot the variation of $\delta = 2\lambda\gamma$ with respect to $\frac{g}{\omega}$ for $\frac{J}{\omega} = 0.2$ and 0.4 in the dimerized phase. It is seen from the figure that for small $\frac{g}{\omega}$ ratio the lattice distortion is almost zero and it increases with the increase of $\frac{g}{\omega}$ or with the decrease of $\frac{J}{\omega}$.

We have also investigated the excitation energy gap (Δ) which is obtained by calculating the lowest excited state energy (ie. lowest energy of the upper band) . In the figure 4. we plot the variation of Δ with respect to $\frac{g}{\omega}$ for $\frac{J}{\omega} = 0.2$ and 0.4. Like the dimerization order parameter, Δ is also very small for small spin-phonon coupling. The result also points to the possibility of gapless spectra for $\frac{g}{\omega} < \frac{g_c}{\omega}$ and gapfull spectra for $\frac{g}{\omega} > \frac{g_c}{\omega}$.

In figure 5. we show the variation of the critical value $\frac{g_c'}{\omega}$ for dimerized to antiferromagnetic phase transition with respect to $\frac{J}{\omega}$. We observe a decrease of $\frac{g_c'}{\omega}$ with the decrease of $\frac{J}{\omega}$ and in the limit $\frac{J}{\omega} \to 0$ the system shows an antiferromagnetic order for any finite spin-phonon coupling. This feature is significantly different if the spin-phonon coupling is treated adiabatically where the ground state of XY model with spin-lattice interaction always represents dimerized phase. Our results signifies that the quantum correction may play a very important role in determining the phases of the ground state of the spin-Peierls systems.

In summary, we have developed a nonadiabatic approach for the interacting spin-phonon problem. We have chosen the Lang-Firsov variational wave function to integrate out the phonon degrees of freedom and obtained an effective spinless fermionic hamiltonian which is solved in the frame work of mean field approximation to calculate the ground state energy, the minimum excitation energy gap and the lattice distortion developed in the ground state. Our investigation indicates two types phase transition one is from spin liquid phase to dimerized phase and another is from dimerized phase to antiferromagnetic phase as we vary the spin-phonon coupling from a very low value. However, these phase transitions are absent if we neglect the quantum lattice fluctuations and treat the problem in the adiabatic approximation. So it is evident that the behavior of spin-Peierls system is significantly modified by quantum lattice fluctuations and an intense investigation is required to explore the effect of nonadiabatic corrections to the spin-Peierls systems. For a realistic calculation of inorganic spin-Peierls system like $CuGeO_3$ one has to study the Heisenberg spin chain with next nearest neighbor frustration .

8

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Figure captions

Figure 1. Variation of the minimum energy (in the unit of the energy of the phonon) with respect to the spin-phonon coupling ($\frac{g}{\omega}$) in the antiferromagnetic phase for J=0.2 (curve a) and J= 0.4 (curve c) and in the dimerized phase for J=0.2 (curve b) and J=0.4 (curve d).

Figure 2. Variation of the dimerized order parameter γ with respect to $\frac{g}{\omega}$ for $J = 0.2$ (curve a) and $J = 0.4$ (curve b) in the dimerized phase.

Figure 3. Variation of the lattice distortion δ with respect to $\frac{g}{\omega}$ in the dimerized phase for $J = 0.2$ (curve a) and $J = 0.4$ (curve b).

Figure 4. The excitation energy gap Δ as a function of $\frac{g}{\omega}$ in the dimerized phase for $J = 0.2$ (curve a) and $J = 0.4$ (curve b).

Figure 5. Variation of the critical value $\frac{g'_c}{\omega}$ for dimerized to antiferromagnetic phase transition with respect to $\frac{J}{\omega}$.
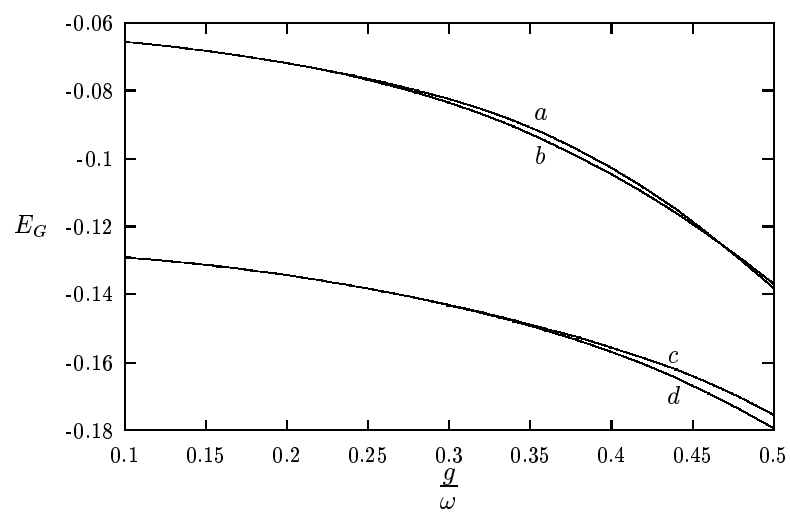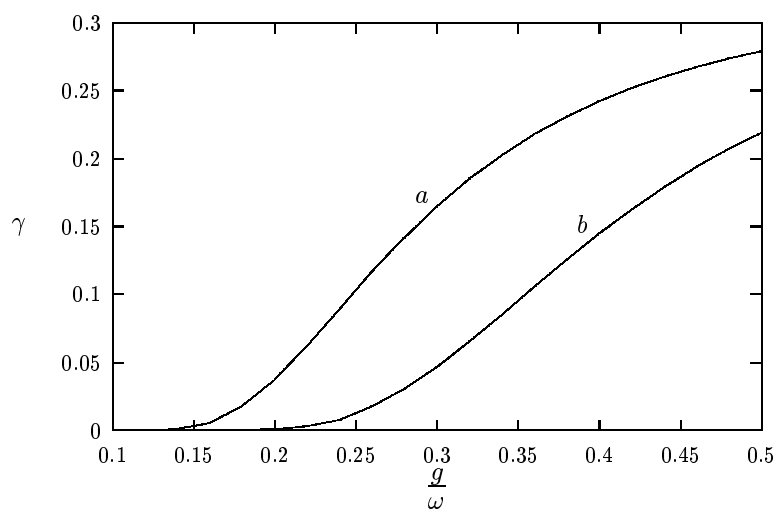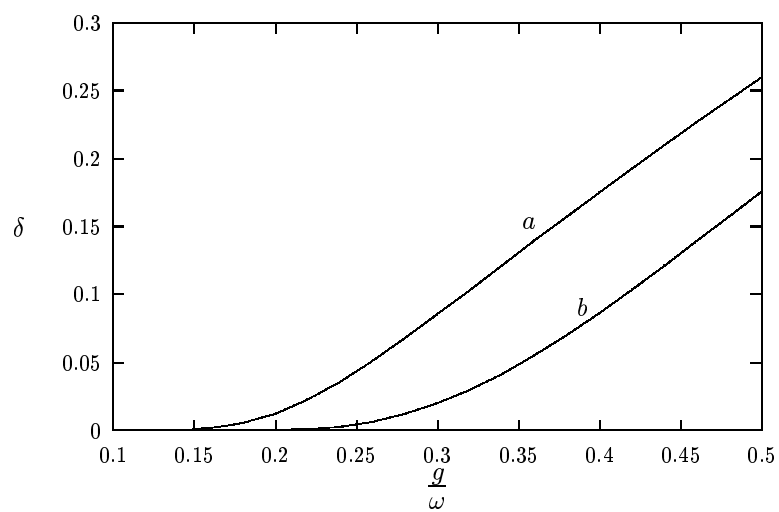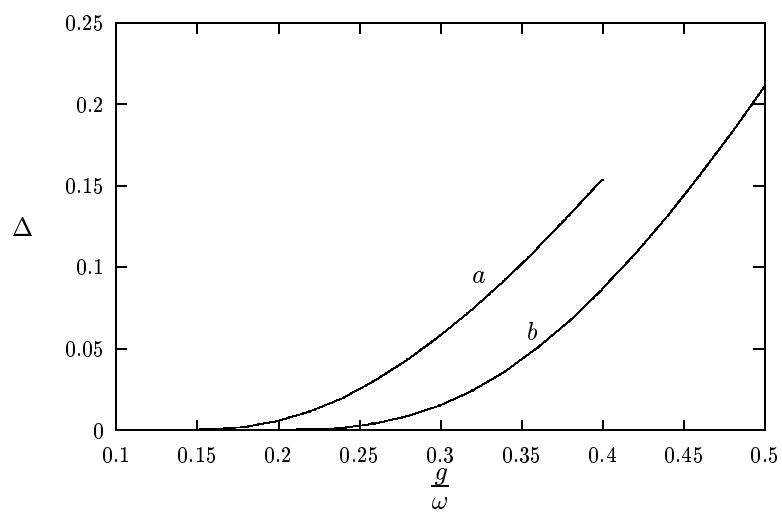
Fig. 1

Fig. 2

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Fig. 4

Fig. 5